Powder Technology 289 (2016) 21–30

Contents lists available at ScienceDirect

Powder Technology

journal homepage: www.elsevier.com/locate/powtec

Effect of roll compactor sealing system designs: A finite element analysis

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ARTICLE INFO

Article history:
Received 1 September 2015
Received in revised form 9 November 2015
Accepted 14 November 2015
Available online 1 December 2015

Keywords:
Roll compaction
Finite Elements Method
Drucker–Prager Cap model
Density distribution
Rimmed-roll

ABSTRACT

In the pharmaceutical industry, the roll compaction is part of the dry granulation process, densifying fine powders into ribbons that will be later milled to produce granules with good flowability for subsequent die compaction process. Roll compactors are constructed with a sealing system, limiting the loss of powder from the sides. However, the sealing system may result in unwanted non-uniformity of the ribbon's properties. In this work, a 3D Finite Elements Method (FEM) modeling is used to analyze the roll compaction process and the effect of sealing system designs on the compacted ribbon's density distribution. A density dependent Drucker–Prager Cap (DPC) constitutive model for microcrystalline cellulose (Avicel PH-101) was calibrated and implemented in Abaqus/Explicit. Two different FEM models were investigated, one with a fixed side sealing called *cheek plates* and another where the side sealing is integrated with the bottom roll called *rimmed-roll*. Both numerical and experimental results clearly show the non-uniform roll pressure and density distribution for the cheek plates assembly, whereas the rimmed-roll shows an overall more uniformly distributed resultant pressure and density distribution. These results demonstrate the capability of FEM modeling to provide insight and help achieving a better understanding of the roll compaction process.

1. Introduction

In the pharmaceutical industry, the roll compaction process is used for dry granulation, densifying fine powders into large dense granular thus improving flowability for direct compression, avoiding segregation in the powder mix and minimizing dust problems [1]. Densifying the powder is done by passing between two counter-rotating rolls, which applies mechanical pressure on the powder. The friction between the feed material and roll surface pushes the powder to a narrow gap, where the powder is subjected to high stresses leading to the formation of compacted ribbons. The roll pressure in the gap region during roll compaction process has the most significant impact on the porosity of the ribbons. Ribbon's density, i.e., solid fraction, is one of the critical quality parameter of roll compaction process that influences the compactibility of granules during tablet formation. The roll compaction system design and operating conditions have a direct effect on the produced compacted ribbon's quality. In order to ensure the consistency, repeatability and quality of the final dosage form, it is important to ensure the quality and avoid heterogeneity of the produced ribbon.

The roll compactors are constructed with a sealing system, limiting the loss of powder from the sides [1,2]. However, the sealing system may result in unwanted non-uniform properties along the ribbon's width and may also exhibit fractured or incomplete compacted edges. Numerous experimental studies were conducted in order to evaluate the density distribution of roll compacted ribbons using destructive and non-destructive methods. The studies were conducted on pharmaceutical powders using laboratory roll compactors integrated with fixed side seals (cheek plates), evaluating the density distribution by ultrasonic[3], micro-indentation[4], X-ray tomography [3,4], near infrared chemical imaging[5,6] and pressure gauges[7,8]. Results showed non-uniformity along the ribbon's width with lower densification at the edges and higher at the middle of the produced ribbon. Moreover, cheek plates may also have a negative effect on the ribbon with fractured or incomplete compacted edges.

Funakoshi [9] developed a roll compactor with concave-convex roll pair in order to avoid the loss of powder and to reduce the ribbon's heterogeneity. The compaction pressure distribution obtained for convaco-convex rolls showed an overall uniform distribution compared to the flat rolls which obtained higher compaction pressure at the middle and lower at the edges. Based on the same mechanics, several roll compactors offers a rimmed-roll sealing system in order to reduce the cheek plates unwanted effects.

Over the past two decades, Finite Elements Method (FEM) modeling were adopted and further developed to simulate pharmaceutical forming processes. FEM models of powder roll compaction process which started considering a plane strain two-dimensional case [10–12], founded to be comparable and more accurate than the one-dimensional analytical Johanson [13] and Slab method[14,15] models. With the increasing computational power in the last years, the development of three-dimensional models provided greater insight on the pressure and density distribution during the roll compaction processes[16,7,17]. Wang et al. [18] found a

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http://dx.doi.org/10.1016/j.powtec.2015.11.039
0032-5910/

variation in the local density for different sealing system using FEM models, however, this numerical study was not fully investigated nor validated experimentally.

The aim of this work is to investigate by FEM modeling the roll compaction process using both rimmed-roll and cheek plates sealing system design. FEM models may give further insight and help understand the mechanics of complex processes such as the roll compaction process. The simulation results are compared with experimentally measured density distribution of the produced ribbons in order to validate the FEM models.

2. Materials and methods

2.1. Roll compaction design and process parameters

The ribbons were produced in this work by Gerteis roll compactor: Mini-pactor 250/25 (Gerteis Machinen + Process engineering AG, Jona, Switzerland). The Gerteis Mini-pactor roll compactor has two possible assemblies for side sealing: cheek plates or rimmed-roll as can be seen in Fig. 1. The most commonly used sealing system is the cheek plates (i.e. fixed side seals), which are fixed and positioned in between the rolls. In order to avoid the problems caused by cheek plates, the Gerteis Mini-pactor also offers a rimmed-roll sealing system. The rimmed-roll is basically a ring, which is mounted on the bottom roll and acts as a sealing in the compaction region. The process parameters set were a controlled gap mode for 1.5 mm, roll speed of 2 rpm and 4 kN/cm roll separation force. The rolls chosen are knurled rolls.

2.2. Powder

The powder used in this work is the microcrystalline cellulose (Avicel PH 101, FMC BioPolymer, Philadelphia, PA, USA). The MCC is one of the most important and widely used excipient in the pharmaceutical industry. It has excellent compressibility properties and used as diluent for drug formulations in the tableting process[19,20]. Tablets with MCC show high strength and on the other hand disintegrate quickly. The true density of the powder blend was determined using a helium pycnometer (Accupyc 1330, Micromeritics Instrument Corp., Norcross, GA, USA) as $\rho_{true} = 1.56$ g/cm^3. The bulk density was obtained from the manufacturer, having values of 0.32 g/cm^3 which correspond to an initial relative density of 0.2. Magnesium stearate (MgSt) was used as lubricant in die compaction.

2.3. Constitutive model

The behavior of the powder, considered as porous compressible material, is described using the density-dependent Drucker–Prager Cap (DPC) model [21]. Assuming the material is isotropic, the model consists of three different parts: A shear failure surface representing shearing flow, a cap surface representing an inelastic hardening for plastic compaction and a transition zone between the two surfaces, providing smooth surface to avoid singularities in the modeling (Fig. 2.). The cap surface serves two main purposes. It bounds the yield surface in pure hydrostatic compression and controls the volume dilatancy when the material yields in shear [22].

Experimental calibration of the DPC model for pharmaceutical [23–28], metallic [29,30] and ceramic [31] powders were extensively conducted in previous studies. The Drucker–Prager shear failure surface can be determined by two of the four experiments for measuring tablets strength: uniaxial tension, pure shear, diametrical compression and uniaxial compression tests. As the maximum loading values of each experiment are positioned on the shear failure line, by using two tests the shear failure line can be determined. The slope of the line represents the friction angle β, and the intersection with q axis represents the cohesion, d. The following equation represents the shear failure line, F_s:

$$F_s = q - d - p\tan\beta = 0. \tag{1}$$

Where the hydrostatic pressure (i.e. negative mean stress), p and the effective Von mises equivalent stress, q are obtained from the stress tensor, σ and defined as follows:

$$p = \frac{1}{3}tr(\sigma) \tag{2}$$

$$q = \sqrt{\frac{1}{2}\left[(\sigma_1-\sigma_2)^2 + (\sigma_2-\sigma_3)^2(\sigma_3-\sigma_1)^2\right]}. \tag{3}$$

The cap yield surface is obtained by analyzing the stress state of the loading and unloading path in die compaction and written as:

$$F_c = \sqrt{(p-P_a)^2 + \left(\frac{Rq}{1+\alpha-\alpha/\cos\beta}\right)^2} - R(d + P_a\tan\beta). \tag{4}$$

Where the density-dependent parameters R, d and β are the cap eccentricity, cohesive strength and internal friction angle, respectively. α is the smoothing transition constant that is used to define the smoothing transition between the shear failure surface and the cap. In this work, an arbitrary transition parameter of $\alpha = 0.01$ was chosen (typically $0.01 < \alpha < 0.05$) in order to ensure avoiding numerical singularities.

As mentioned previously, in order to obtain a smoothing transition between the shear failure surface and the cap yield surface, a transition surface F_t should be applied:

$$F_t = \sqrt{(p-P_a)^2 + \left[q - \left(1 - \frac{\alpha}{\cos\beta}\right)(d + P_a\tan\beta)\right]^2} - \alpha(d + P_a\tan\beta). \tag{5}$$

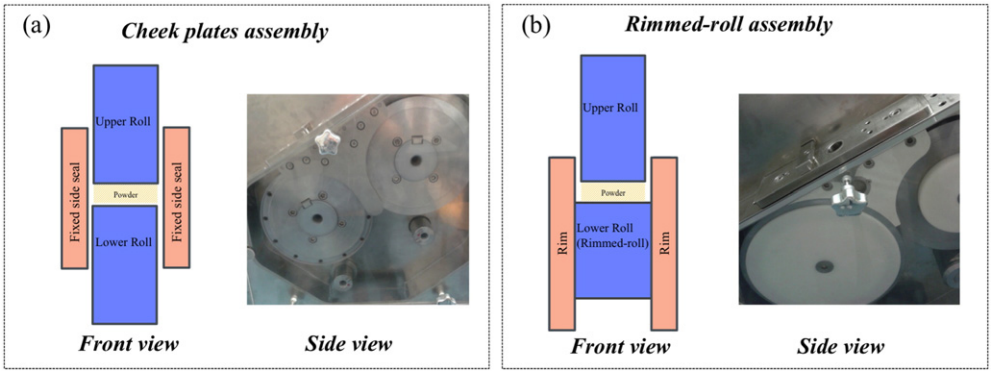

Fig. 1. Gerteis Minipactor's possible side seal assemblies a) cheek plates and b) rimmed-roll.